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Title:

Describing non-adiabatic quantum effects in large dimensional systems

Abstract:

During non-adiabatic dynamics (NAD), nuclei are strongly coupled to electrons. Conical intersections (CIs) are features of the adiabatic energies that exhibit these strong couplings. They induce subtle quantum effects that can be used to elaborate new control strategies. In this context, theoretical approaches are used to understand details at the atomic level and to test control schemes. Involved quantum effects imply to use a full quantum approach for simulating the dynamics. Hence, obtaining a Hamiltonian is a prerequisite for further investigations.

Nowadays, NAD are routinely simulated for studying the spectroscopy of molecules containing up to 20 atoms [1] by fitting Hamiltonian models and using the MCTDH method [2]. Obtaining models for larger systems is currently a bottleneck. I will present strategies for obtaining such models and simulating dynamics of larger systems (20 to 70 atoms) going beyond spectroscopic applications (reactivity) [3]. I will also discuss a specific interference effect caused by the Berry phase appearing at CIs [4].

[1] S. Kopec et al., J. Chem. Phys. 144, 024314 (2016); G. Wu et al., J. Chem. Phys. 142, 074302 (2015)
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[3] L. Joubert-Doriol et al., J. Chem. Phys. 140, 044301 (2014); J. S. Endicott et al., J. Chem. Phys. 141, 034104 (2014); L. Joubert-Doriol et al., ArXiv: 1602.05044 (2016)
[5] L. Joubert-Doriol et al., J. Chem. Phys. 139, 234103 (2013)